$\LaTeX$ command declarations here.

In [6]:

```
from __future__ import division

# plotting
%matplotlib inline
from matplotlib import pyplot as plt;
import matplotlib as mpl;
from mpl_toolkits.mplot3d import Axes3D

# scientific
import numpy as np;
import sklearn as skl;
import sklearn.datasets;
import sklearn.cluster;
import sklearn.mixture;

# ipython
import IPython;

# python
import os;
import random;

##########################################################

# image processing
import PIL;

# trim and scale images
def trim(im, percent=100):
    print("trim:", percent);
    bg = PIL.Image.new(im.mode, im.size, im.getpixel((0,0)))
    diff = PIL.ImageChops.difference(im, bg)
    diff = PIL.ImageChops.add(diff, diff, 2.0, -100)
    bbox = diff.getbbox()
    if bbox:
        x = im.crop(bbox)
        return x.resize(((x.size[0]*percent)//100,
                         (x.size[1]*percent)//100),
                        PIL.Image.ANTIALIAS);


#########################################################

# daft (rendering PGMs)
import daft;

# set to FALSE to load PGMs from static images
RENDER_PGMS = True;

# decorator for pgm rendering
def pgm_render(pgm_func):
    def render_func(path, percent=100, render=None, *args, **kwarg
s):
        print("render_func:", percent);
```

```
        # render
        render = render if (render is not None) else RENDER_PGMS;

        if render:
            print("rendering");
            # render
            pgm = pgm_func(*args, **kwargs);
            pgm.render();
            pgm.figure.savefig(path, dpi=300);

            # trim
            img = trim(PIL.Image.open(path), percent);
            img.save(path, 'PNG');
        else:
            print("not rendering");

        # error
        if not os.path.isfile(path):
            raise Exception("Error:  Graphical model image %s not f
ound.  \
            You may need to set RENDER_PGMS=True." % path);

        # display
        return IPython.display.Image(filename=path);
    return render_func;

##########################################################
```

EECS 545: Machine Learning

Lecture 19: Unsupervised Learning (PCA & ICA)

- Instructor: **Jacob Abernethy**
- Date: March 28, 2016

Lecture Exposition: Saket

References

- **[MLAPP]** Murphy, Kevin. *Machine Learning: A Probabilistic Perspective* (https://mitpress.mit.edu/books/machine-learning-0). 2012.
- **[PRML]** Bishop, Christopher. *Pattern Recognition and Machine Learning* (http://research.microsoft.com/en-us/um/people/cmbishop/prml/). 2006.

Outline

- Probabilistic Component Analysis
  - Classical View
  - Probabilistic PCA
- Independent Components Analysis
  - Cocktail Party Problem

Principal Components Analysis

> Uses material from **[MLAPP]** and **[PRML]**

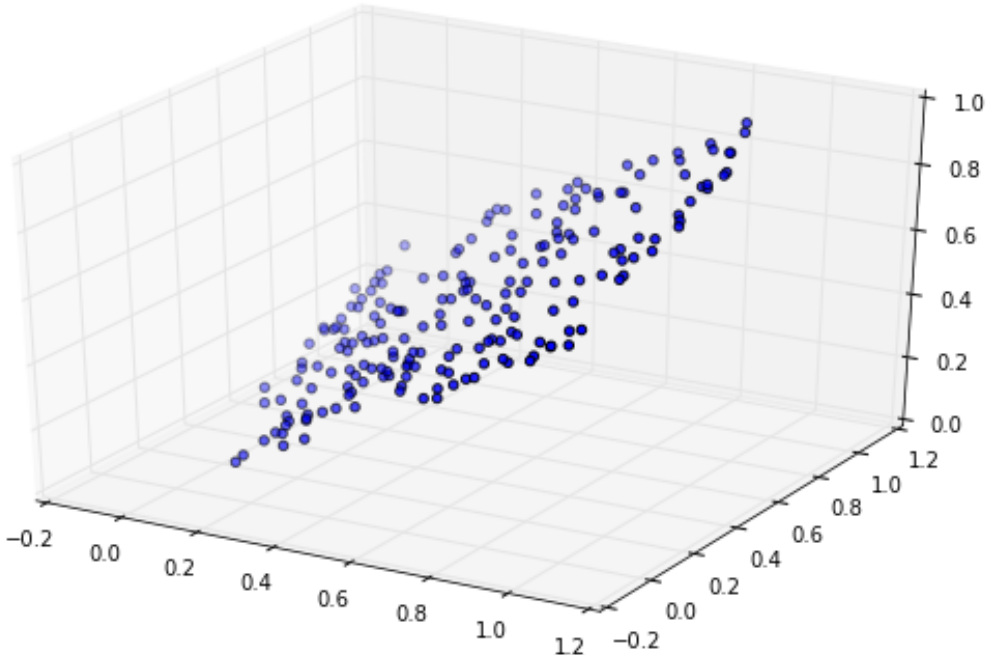
Dimensionality Reduction

High-dimensional data may have **low-dimensional structure**.

- We only need two dimensions to describe a rotated plane in 3d!

In [34]:
```
def plot_plane():
    # random samples
    n = 200;
    data = np.random.random((3,n));
    data[2,:] = 0.4 * data[1,:] + 0.6 * data[0,:];

    # plot plane
    fig = plt.figure(figsize=(10,6));
    ax = fig.add_subplot(111, projection="3d");
    ax.scatter(*data);
```

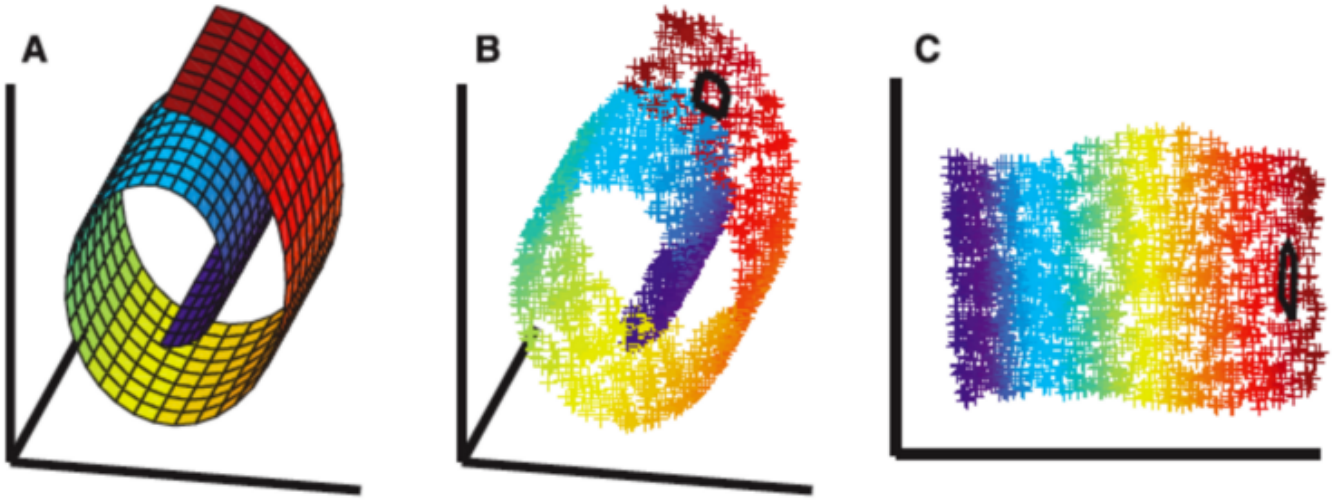
```
In [36]: plot_plane()
```



Dimensionality Reduction

Data may even be embedded in a low-dimensional **nonlinear manifold**.

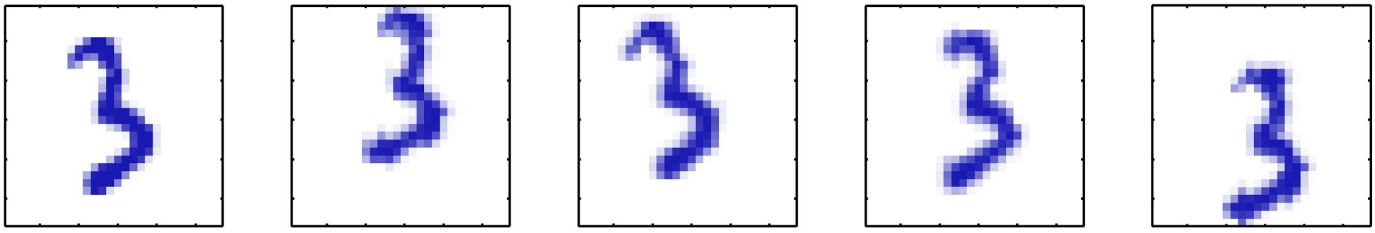
- How can we recover a low-dimensional representation?



Dimensionality Reduction

As an even more extreme example, consider a dataset consisting of the same image translated and rotate in different directions:

- Only 3 degrees of freedom for a 100x100-dimensional dataset!



Principal Components Analysis

Given a set $X = \{x_n\}$ of observations

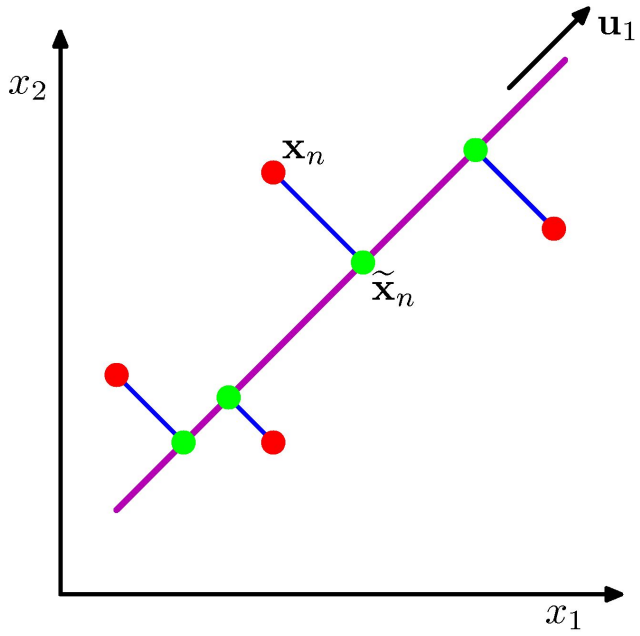
- in a space of dimension D,
- find a **linear subspace** of dimension $M < D$
- that captures most of its variability.

PCA can be described in two equivalent ways:

- maximizing the variance of the projection, or
- minimizing the squared approximation error.

PCA: Equivalent Descriptions

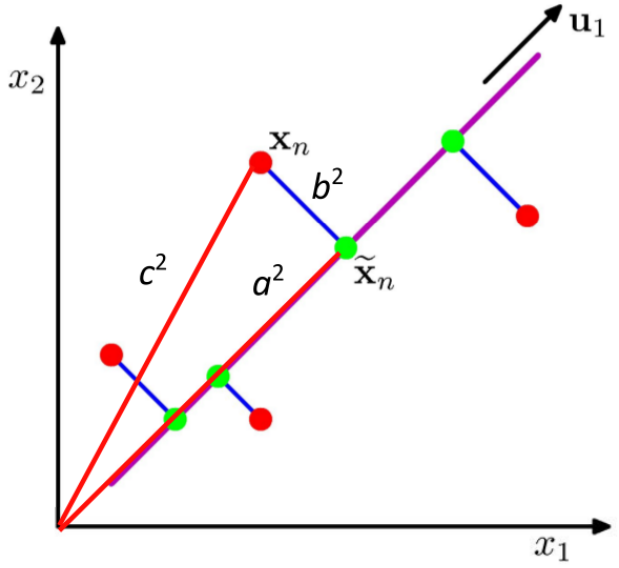
Maximize variance or minimize squared projection error:



PCA: Equivalent Descriptions

With mean at the origin $c_i^2 = a_i^2 + b_i^2$, with constant c_i^2

- Minimizing b_i^2 maximizes a_i^2 and vice versa



PCA: First Principal Component

Given data points $\{x_n\}$ in D-dim space.

- Mean $\bar{x} = \frac{1}{N} \sum_{n=1}^{N} x_n$
- Data covariance ($D \times D$ matrix): $S = \frac{1}{N} \sum_{n=1}^{N} (x_n - \bar{x})(x_n - \bar{x})^T$

Let u_1 be the **principal component** we want.

- Unit length $u_1^T u_1 = 1$
- Projection of x_n is $u_1^T x_n$

PCA: First Principal Component

Goal: Maximize the projection variance over directions u_1:

$$\frac{1}{N}\sum_{n=1}^{N}\{u_1^T x_n - u_1^T \bar{x}\}^2 = u_1^T S u_1$$

- Use a Lagrange multiplier to enforce $u_1^T u_1 = 1$
  - Maximize: $u_1^T S u_1 + \lambda(1 - u_1^T u_1)$
- Derivative is zero when $Su_1 = \lambda u_1$
  - That is, $u_1^T S u_1 = \lambda$
- So u_1 is eigenvector of S with largest eigenvalue.

PCA: Maximizing Variance

The top M eigenvectors of the empirical covariance matrix S give the M principal components of the data.

- Minimizes squared projection error
- Maximizes projection variances

Recall: These are the top M left singular vectors of the data matrix $\hat{X}$, where $\hat{X} := X - \bar{x}1_N$, i.e. we shift X to ensure 0-mean rows.

- c.f. Homework 1

Example: Eigenfaces

Images from www.cse.unr.edu/~bebis/CS485/Lectures/Eigenfaces.ppt

Example: Face Recognition via Eigenfaces

In [39]:

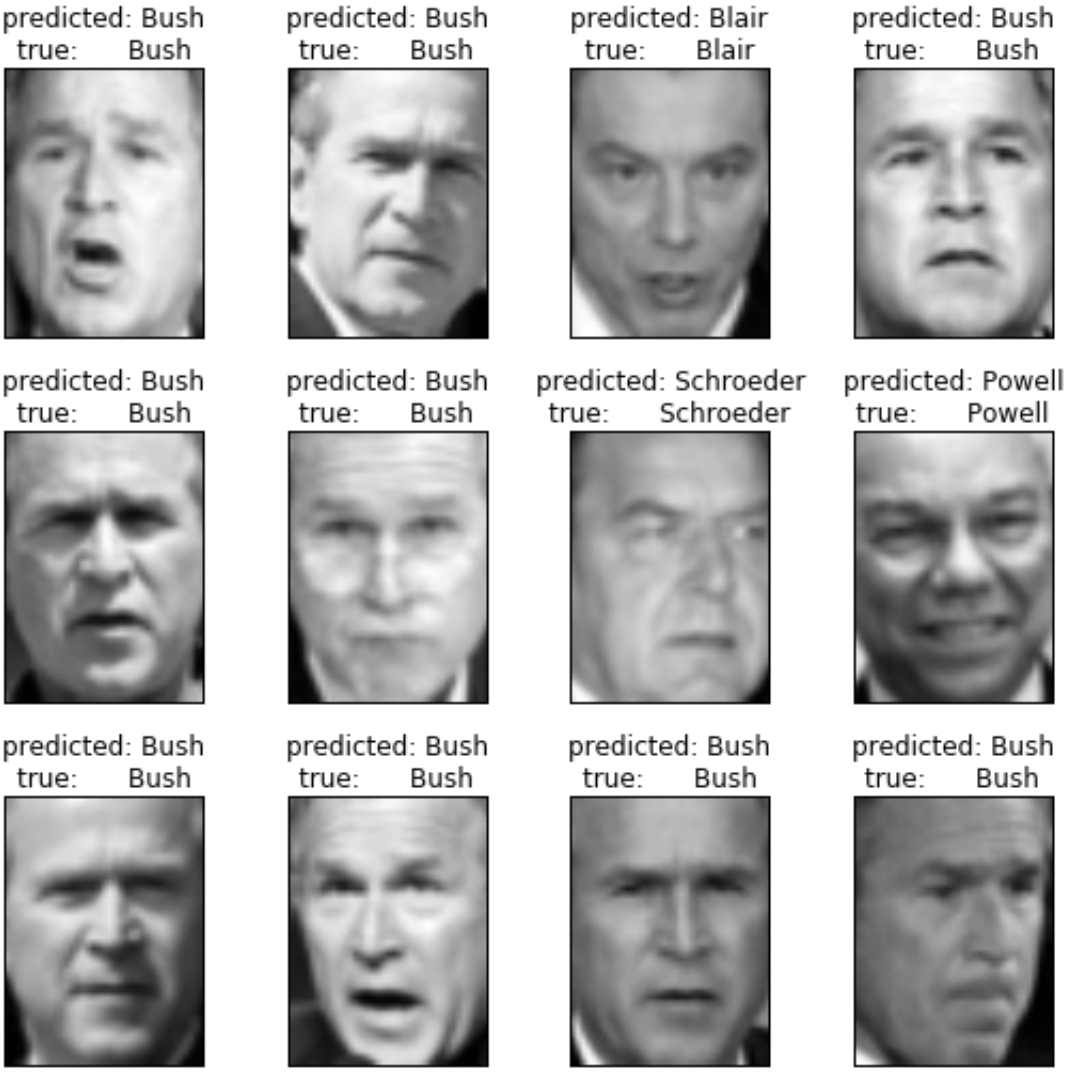
```
## scikit example: Faces recognition example using eigenfaces and S
VMs

from __future__ import print_function

from time import time
import matplotlib.pyplot as plt

from sklearn.cross_validation import train_test_split
from sklearn.datasets import fetch_lfw_people
from sklearn.grid_search import GridSearchCV
from sklearn.metrics import classification_report
from sklearn.metrics import confusion_matrix
from sklearn.decomposition import RandomizedPCA
from sklearn.svm import SVC


###############################################################################
# Download the data, if not already on disk and load it as numpy ar
rays

lfw_people = fetch_lfw_people(min_faces_per_person=70, resize=0.4)

# introspect the images arrays to find the shapes (for plotting)
n_samples, h, w = lfw_people.images.shape

# for machine learning we use the 2 data directly (as relative pixe
l
# positions info is ignored by this model)
X = lfw_people.data
n_features = X.shape[1]

# the label to predict is the id of the person
y = lfw_people.target
target_names = lfw_people.target_names
n_classes = target_names.shape[0]


###############################################################################
# Split into a training set and a test set using a stratified k fol
d

# split into a training and testing set
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.25, random_state=42)


###############################################################################
# Compute a PCA (eigenfaces) on the face dataset (treated as unlabe
led
# dataset): unsupervised feature extraction / dimensionality reduct
```

```
ion
n_components = 150

#print("Extracting the top %d eigenfaces from %d faces"
#      % (n_components, X_train.shape[0]))
#t0 = time()
pca = RandomizedPCA(n_components=n_components, whiten=True).fit(X_t
rain)
#print("done in %0.3fs" % (time() - t0))

eigenfaces = pca.components_.reshape((n_components, h, w))

#print("Projecting the input data on the eigenfaces orthonormal bas
is")
#t0 = time()
X_train_pca = pca.transform(X_train)
X_test_pca = pca.transform(X_test)
#print("done in %0.3fs" % (time() - t0))


###############################################################################
# Train a SVM classification model

#print("Fitting the classifier to the training set")
#t0 = time()
param_grid = {'C': [1e3, 5e3, 1e4, 5e4, 1e5],
              'gamma': [0.0001, 0.0005, 0.001, 0.005, 0.01, 0.1], }
clf = GridSearchCV(SVC(kernel='rbf', class_weight='balanced'), para
m_grid)
clf = clf.fit(X_train_pca, y_train)
#print("done in %0.3fs" % (time() - t0))
#print("Best estimator found by grid search:")
#print(clf.best_estimator_)


###############################################################################
# Quantitative evaluation of the model quality on the test set

#print("Predicting people's names on the test set")
#t0 = time()
y_pred = clf.predict(X_test_pca)
#print("done in %0.3fs" % (time() - t0))

#print(classification_report(y_test, y_pred, target_names=target_na
mes))
#print(confusion_matrix(y_test, y_pred, labels=range(n_classes)))


###############################################################################
# Qualitative evaluation of the predictions using matplotlib
```

```
def plot_gallery(images, titles, h, w, n_row=3, n_col=4):
    """Helper function to plot a gallery of portraits"""
    plt.figure(figsize=(1.8 * n_col, 2.4 * n_row))
    plt.subplots_adjust(bottom=0, left=.01, right=.99, top=.90, hsp
ace=.35)
    for i in range(n_row * n_col):
        plt.subplot(n_row, n_col, i + 1)
        plt.imshow(images[i].reshape((h, w)), cmap=plt.cm.gray)
        plt.title(titles[i], size=12)
        plt.xticks(())
        plt.yticks(())


# plot the result of the prediction on a portion of the test set

def title(y_pred, y_test, target_names, i):
    pred_name = target_names[y_pred[i]].rsplit(' ', 1)[-1]
    true_name = target_names[y_test[i]].rsplit(' ', 1)[-1]
    return 'predicted: %s\ntrue:      %s' % (pred_name, true_name)

prediction_titles = [title(y_pred, y_test, target_names, i)
                     for i in range(y_pred.shape[0])]
```

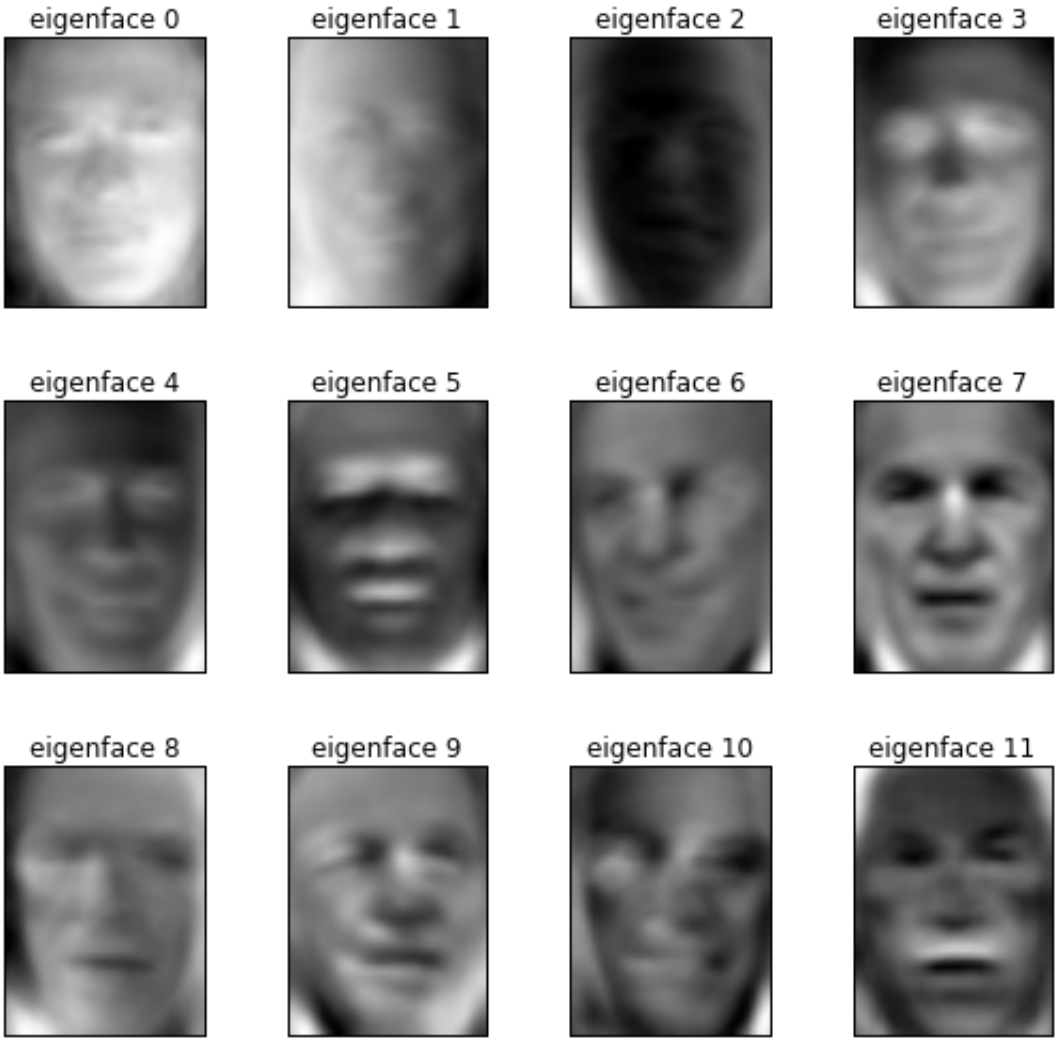
```
/home/ben/anaconda3/lib/python3.5/site-packages/sklearn/externals/
joblib/func_inspect.py:191: DeprecationWarning: inspect.getargspec
() is deprecated, use inspect.signature() instead
  arg_spec = inspect.getargspec(func)
```

In [40]:
```
plot_gallery(X_test, prediction_titles, h, w)
```



Example: Face Recognition

In [42]:
```
eigenface_titles = ["eigenface %d" % i for i in range(eigenfaces.shape[0])]
plot_gallery(eigenfaces, eigenface_titles, h, w)
```



Probabilistic PCA

We can view PCA as solving a probabilistic **latent variable** problem.

$$x = Wz + \mu + \epsilon$$
$$z \sim \mathcal{N}(0, I_M)$$

where we describe

- data $x \in \mathbb{R}^D$ in terms of
- latent variable $z \in \mathbb{R}^M$ in lower dimensional space, via
- linear transformation $W \in \mathbb{R}^{D \times M}$ that maps $x \mapsto z$
- and ϵ is a D-dimensional zero-mean Gaussian-distributed noise variable with covariance $\sigma^2 I$.

Probabilistic PCA

Given the generative model

$$x = Wz + \mu + \epsilon$$

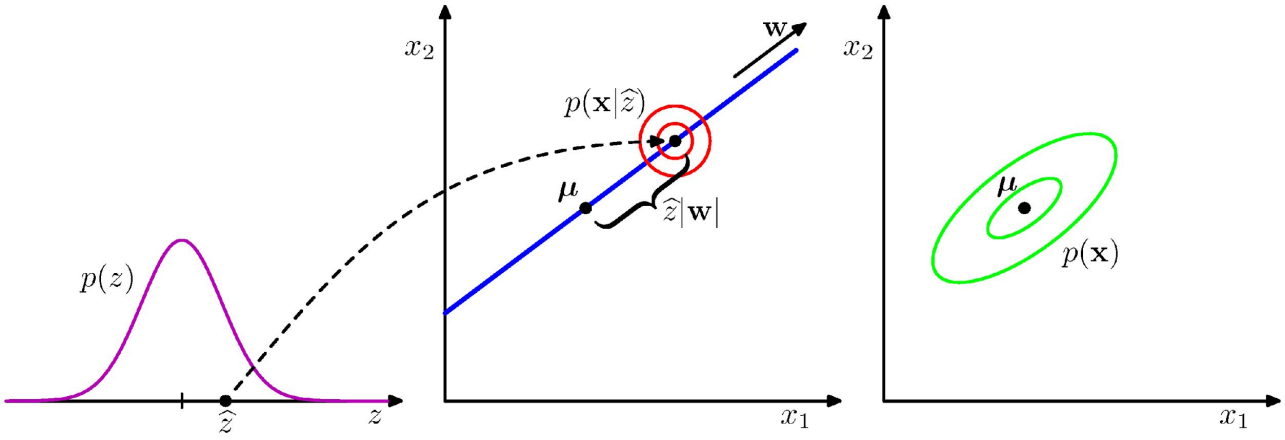
we can infer

$$\mathbb{E}[x] = \mathbb{E}[Wz + \mu + \epsilon] = \mu$$

$$\begin{aligned}\text{Cov}[x] &= \mathbb{E}[(Wz + \epsilon)(Wz + \epsilon)^T] \\ &= \mathbb{E}[(Wzz^TW^T] + \mathbb{E}[\epsilon\epsilon^T] \\ &= WW^T + \sigma^2 I\end{aligned}$$

Probabilistic PCA

$$x = Wz + \mu + \epsilon$$



Probabilistic PCA: Likelihood

- (Marginal) likelihood

$$\begin{aligned}\log p(X|\mu, W, \sigma^2) &= \sum_n \log p(x_n|W, \mu, \sigma^2) \\ &= -\frac{ND}{2}\log 2\pi - \frac{N}{2}\log|C| - \frac{1}{2}\sum_n (x_n - \mu)^T C^{-1}(x_n - \mu)\end{aligned}$$

$$C = WW^T + \sigma^2 I$$

- We can simply maximize this likelihood function with respect to μ, W, σ.

Probabilistic PCA: Maximum Likelihood

- Mean: $\mu = \bar{x}$
- Noise: $\sigma^2_{ML} = \frac{1}{D-M} \sum_{i=M+1}^{D} \lambda_i$
- W: $W_{ML} = U_M (L_M - \sigma^2 I)^{\frac{1}{2}} R$

where L_M is diag with the M largest eigenvalues and U_M is the M corresponding eigenvectors And R is an arbitrary $M \times M$ rotation (i.e., z can be defined by rotating "back")

Probabilistic PCA: Expectation Maximization

- Latent variable model

$$p(z) = \mathcal{N}(z|0, I)$$

$$p(x|z) = \mathcal{N}(x|Wz + \mu, \sigma^2 I)$$

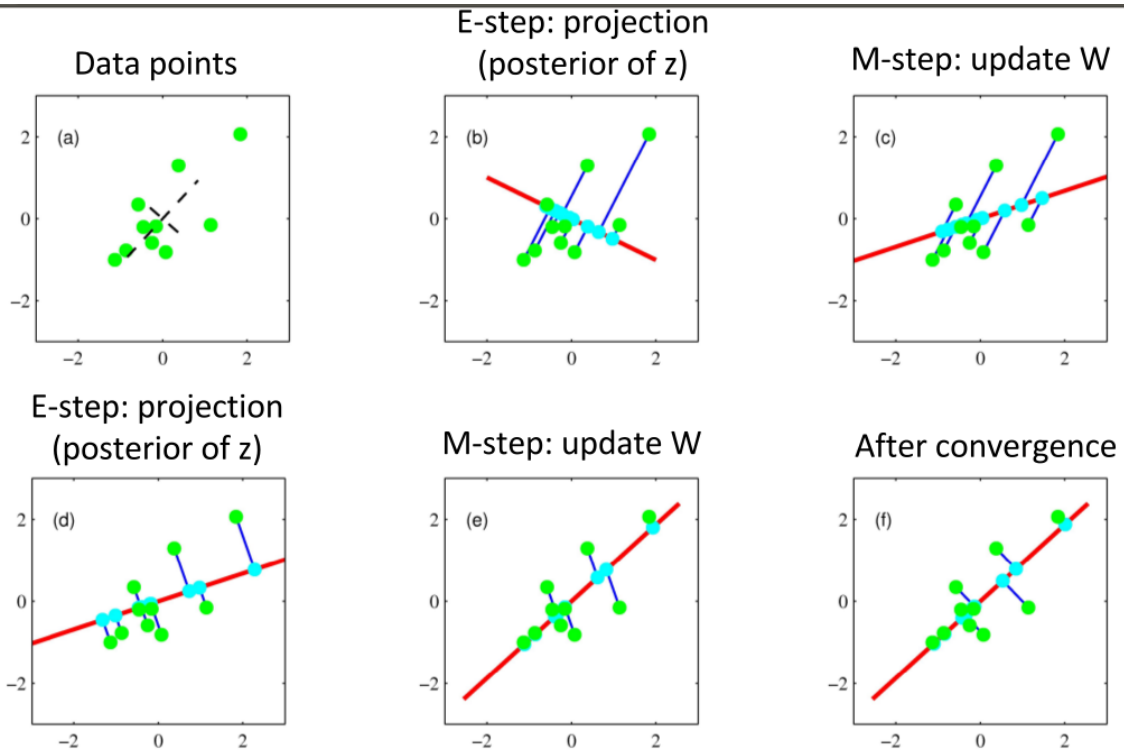
- E-step: Estimate the posterior $q(z) = P(z|x)$
  - Use linear Gaussian
- M-step: Maximize the data-completion likelihood given $q(z)$:

$$\max_{\theta=\{\mu,W,\sigma\}} \quad \sum_i \sum_{z^{(i)}} q(z^{(i)}) \log P_\theta(x^{(i)}, z^{(i)})$$

PPCA: Advantages of EM over SVD

- EM can be **faster**. In particular, assuming $N, D \gg L$, the dominant cost of EM is the projection operation in the E step, so the overall time is $O(TLND)$, where T is the number of iterations.
- EM can be implemented in an **online** fashion, i.e., we can update our estimate of W as the data streams in.
- EM can handle **missing data** in a simple way.
- EM can be extended to handle **mixtures of PPCA/ FA models**.
- EM can be modified to **variational EM** or to variational Bayes EM to fit more complex models.

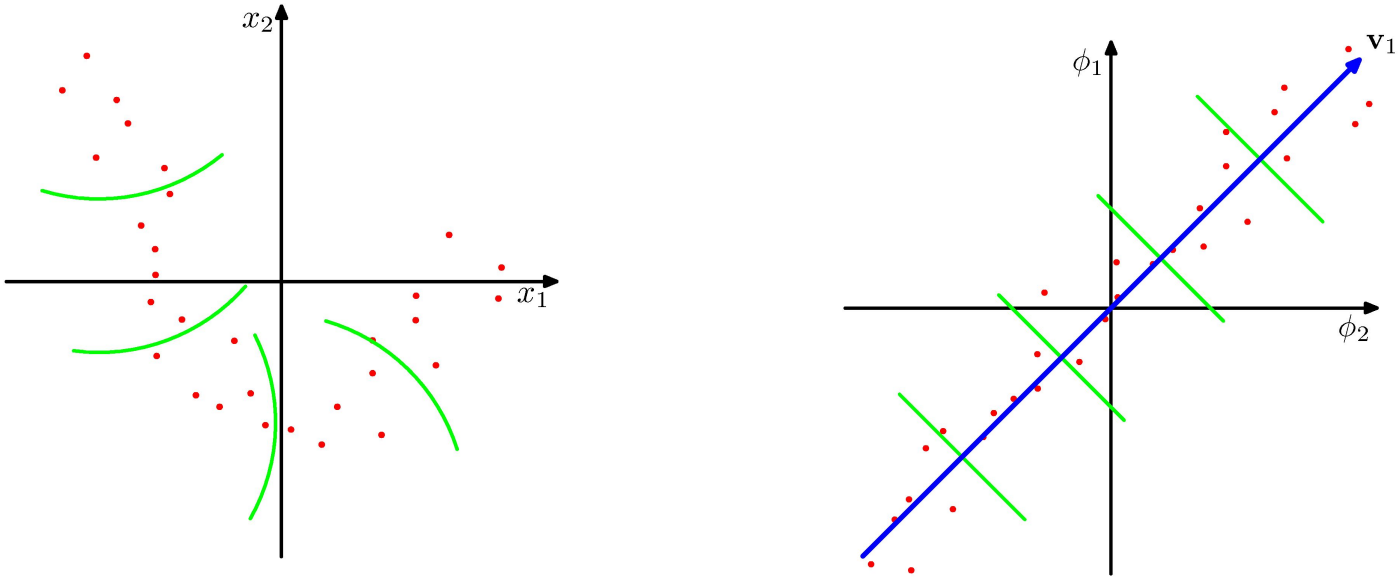
Probabilistic PCA: Expectation Maximization



Break time!

Kernel PCA

Suppose the regularity that allows dimensionality reduction is non-linear.



Kernel PCA

- As with regression and classification, we can transform the raw input data {xn} to a set of feature values

$$\{x_n\} \rightarrow \{\phi(x_n)\}$$

- Linear PCA (on the nonlinear feature space) gives us a linear subspace in the feature value space, corresponding to nonlinear structure in the data space.

Kernel PCA

- Define a kernel, to avoid having to evaluate the feature vectors explicitly.

$$\kappa(x, x') = \phi(x)^T \phi(x')$$

- Define the Gram matrix K of pairwise similarities among the data points:

$$K_{nm} = \phi(x_n)^T \phi(x_m) = \kappa(x_n, x_m)$$

- Express PCA in terms of the kernel,
  - Some care is required to centralize the data.

Independent Components Analysis

> Uses material from **[MLAPP]** and **[PRML]**

Independent Component Analysis

Suppose N independent signals are mixed, and sensed by N independent sensors.

- Cocktail party with speakers and microphones.
- EEG with brain wave sources and sensors.

> Can we reconstruct the original signals, given the mixed data from the sensors?

Independent Component Analysis

The sourcess must be independent.

- And they **must be non-Gaussian**.
- If Gaussian, then there is no way to find unique independent components.

Linear mixing to get the sensor signals x.

- $\boldsymbol{x} = \boldsymbol{A}\boldsymbol{s}$
- or $\boldsymbol{s} = \boldsymbol{W}\boldsymbol{x}$ (i.e., $\boldsymbol{W} = \boldsymbol{A}^{-1}$)

$\boldsymbol{A}$ are the **bases**, $\boldsymbol{W}$ are the **filters**

ICA: Algorithm

- There are several formulations of ICA:
  - Maximum likelihood
  - Maximizing non-Gaussianity (popular)

- Common steps of ICA (e.g., FastICA):
  - Apply PCA whitening (aka sphering) to the data
  - Find orthogonal unit vectors along which the that non-Gaussianity are maximized

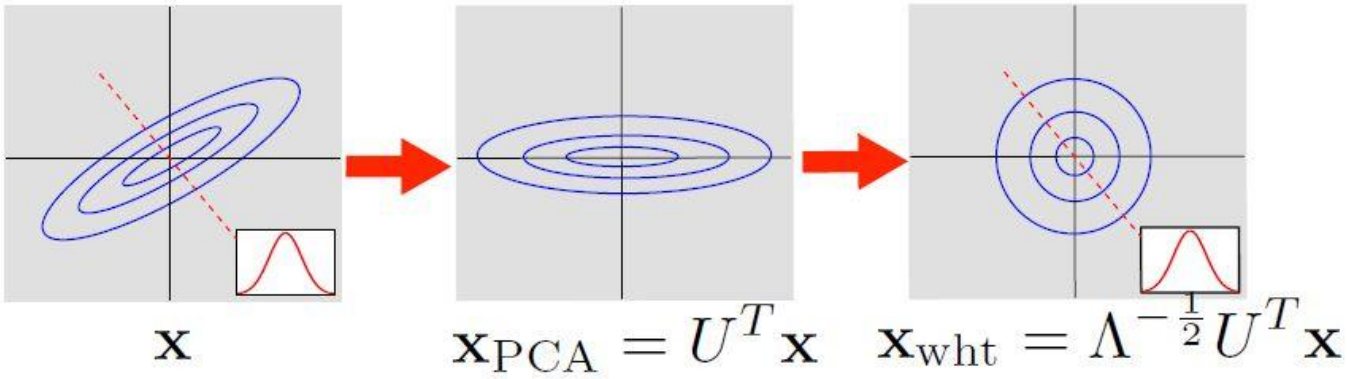
$$\max_{W} \quad f(W\tilde{x}) \qquad s.t. \quad WW^T = I$$

where f(x) can be “kurtosis”, L1 norm, etc.

ICA: Step 1, Preprocessing

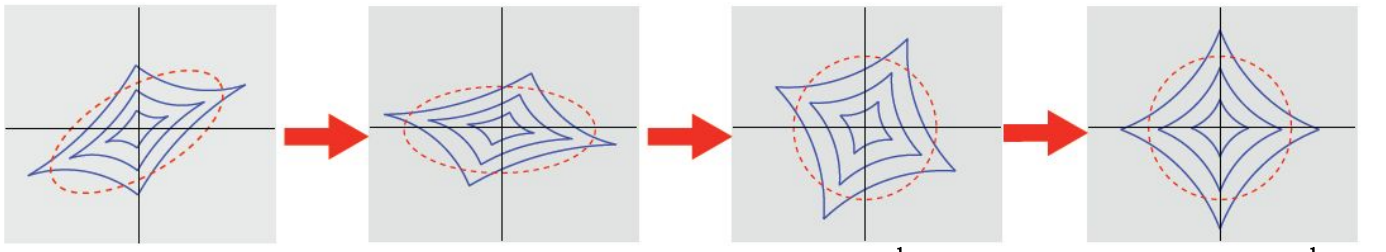
We use **PCA Whitening** to preprocess the data:

- Apply PCA: $\Sigma = U\Lambda U^T$
- Project (rotate) to the principal components
- “Scale” each axis so that the transformed data has identity as covariance.



ICA: Step 2, Maximize Non-Gaussianity

Rotate to maximize non-Gaussianity

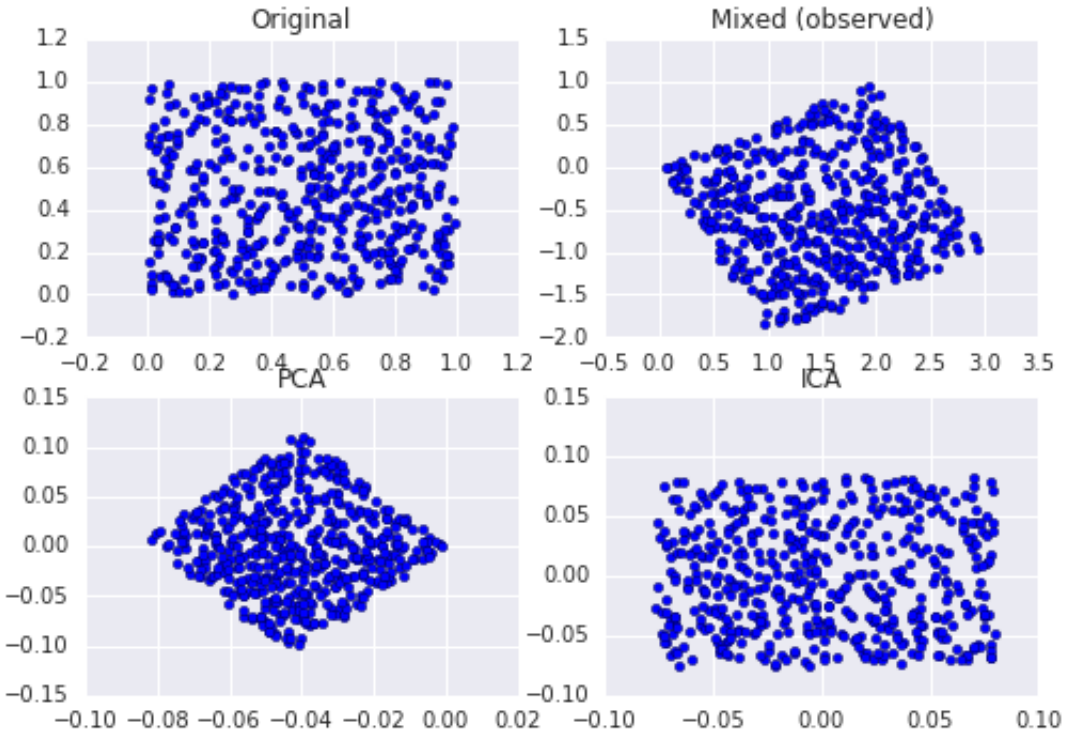


x $x_{PCA} = U^T x$ $x_{PCA} = \Lambda^{-\frac{1}{2}} U^T x$ $x_{ICA} = V \Lambda^{-\frac{1}{2}} U^T x$

ICA vs PCA

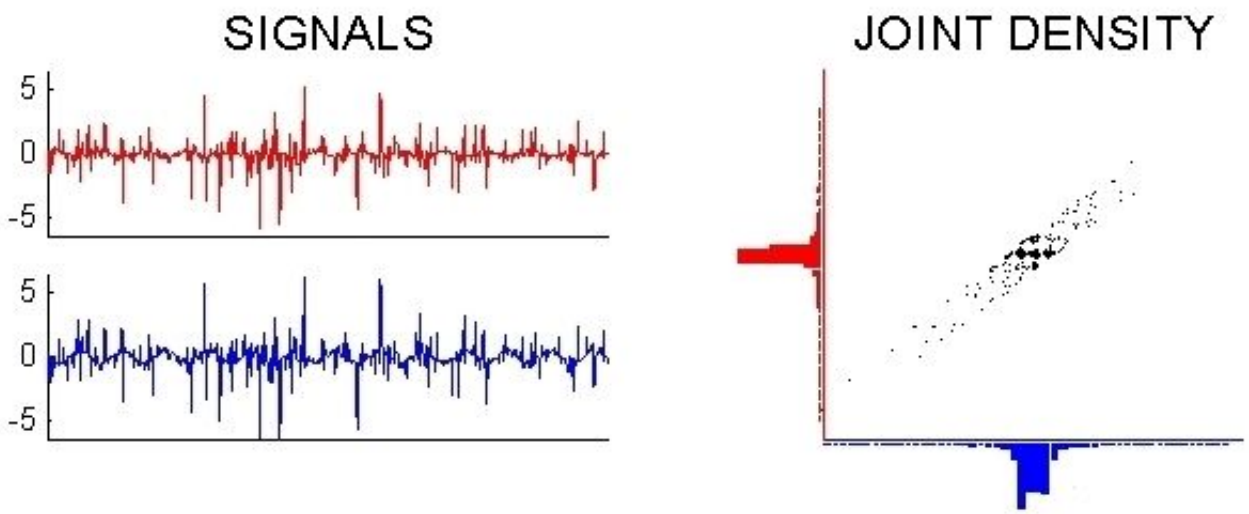
In [46]:
```
from __future__ import division
import numpy as np
from sklearn.decomposition import FastICA
from matplotlib import pyplot as plt
import seaborn;

# thanks to Daniel LeJeune for the code!
def plot_ica_pca():

    # original samples
    S = np.random.rand(2,500)
    plt.subplot(2,2,1)
    plt.scatter(S[0,:], S[1,:])
    plt.title('Original')

    # observed samples
    A = np.array([[1, 2], [-2, 1]])
    X = A.dot(S)
    plt.subplot(2,2,2)
    plt.scatter(X[0,:], X[1,:])
    plt.title('Mixed (observed)')

    # PCA recovered samples
    _,_,V = np.linalg.svd(X)
    plt.subplot(2,2,3)
    plt.scatter(V[0,:], V[1,:])
    plt.title('PCA')

    # ICA recovered samples
    fica = FastICA()
    Y = fica.fit_transform(X.T).T
    plt.subplot(2,2,4)
    plt.scatter(Y[0,:], Y[1,:])
    plt.title('ICA')
```

In [47]:
```
plot_ica_pca()
```



ICA: Mixture Example

Input Signals and Density



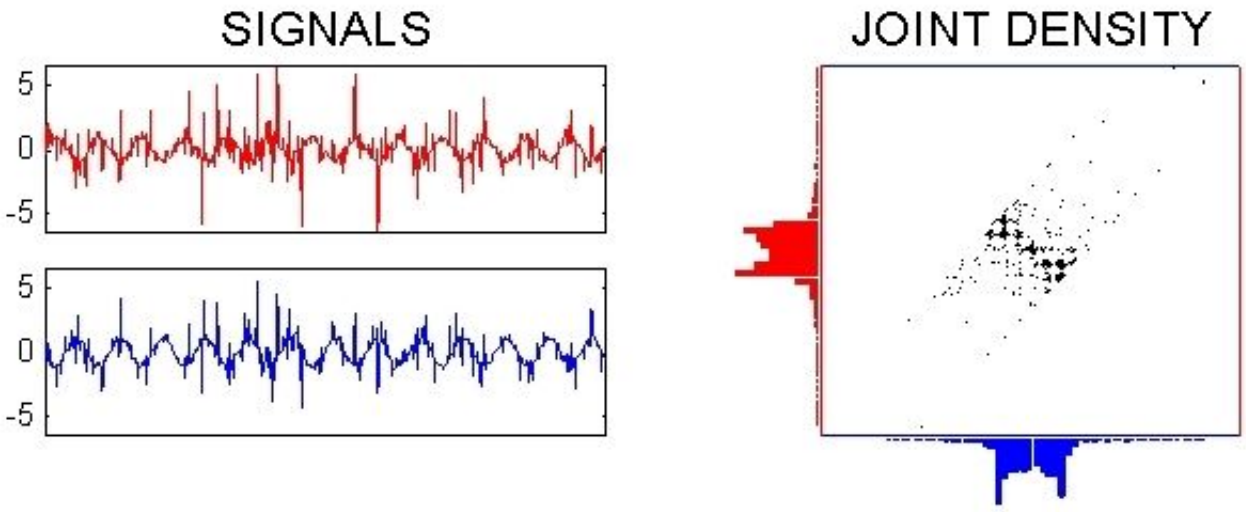
Input signals and density

ICA: Mixture Example

To whiten the input data:

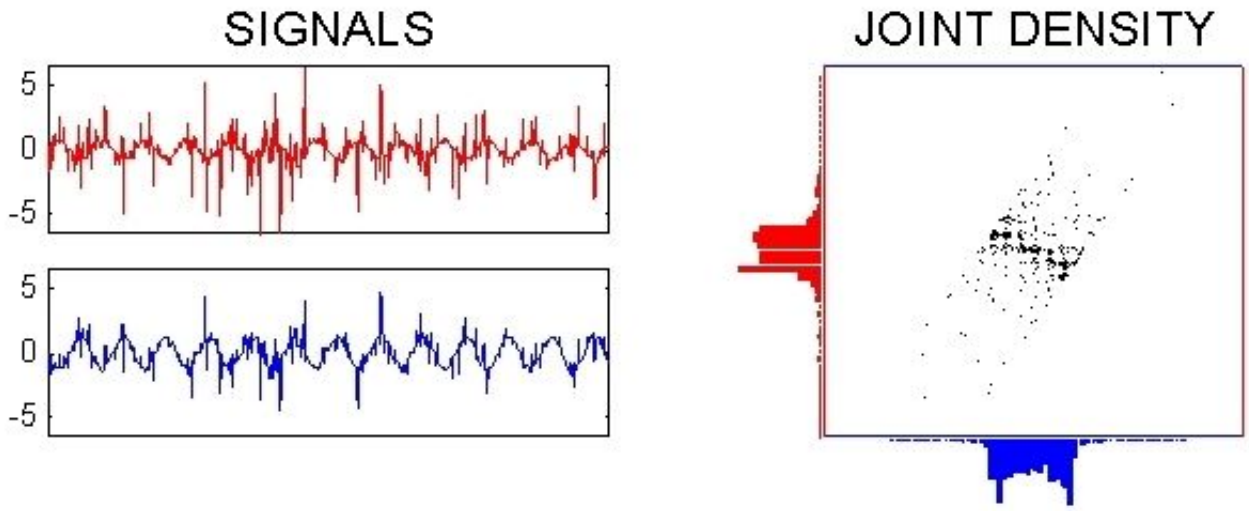
- We want a linear transformation $\boldsymbol{y} = V\boldsymbol{x}$
- So the components are uncorrelated: $\mathbb{E}[\boldsymbol{y}\boldsymbol{y}^T] = I$
- Given the original covariance $C = \mathbb{E}[\boldsymbol{x}\boldsymbol{x}^T]$
- We can use $V = C^{-\frac{1}{2}}$
- Because $\mathbb{E}[\boldsymbol{y}\boldsymbol{y}^T] = \mathbb{E}[V\boldsymbol{x}\boldsymbol{x}^T V^T] = C^{-\frac{1}{2}} C C^{-\frac{1}{2}} = I$

ICA: Mixture Example



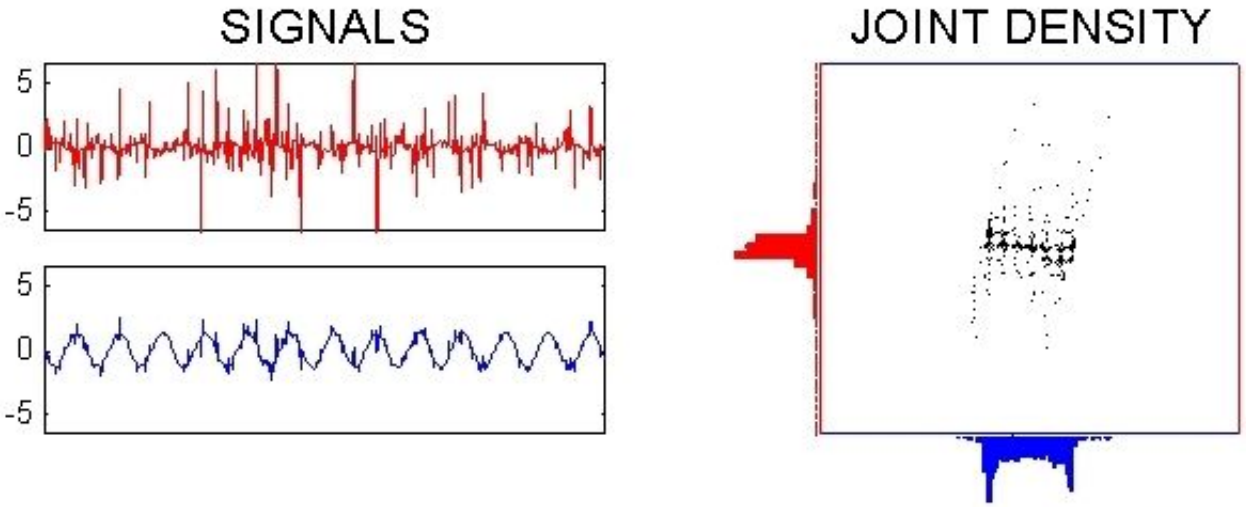
Separated signals after 1 step of FastICA

ICA: Mixture Example



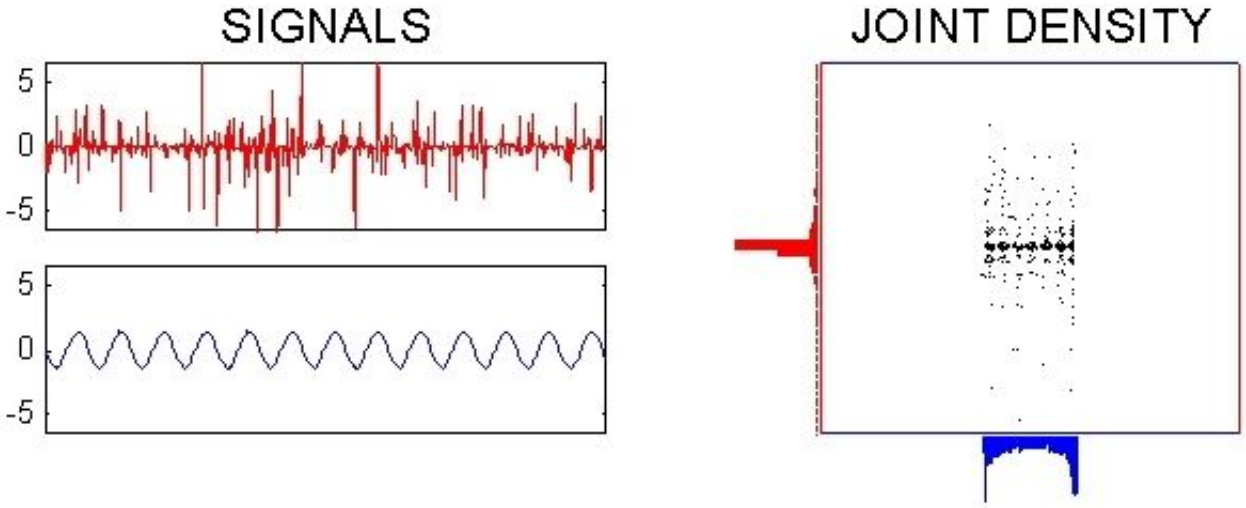
Separated signals after 2 steps of FastICA

ICA: Mixture Example



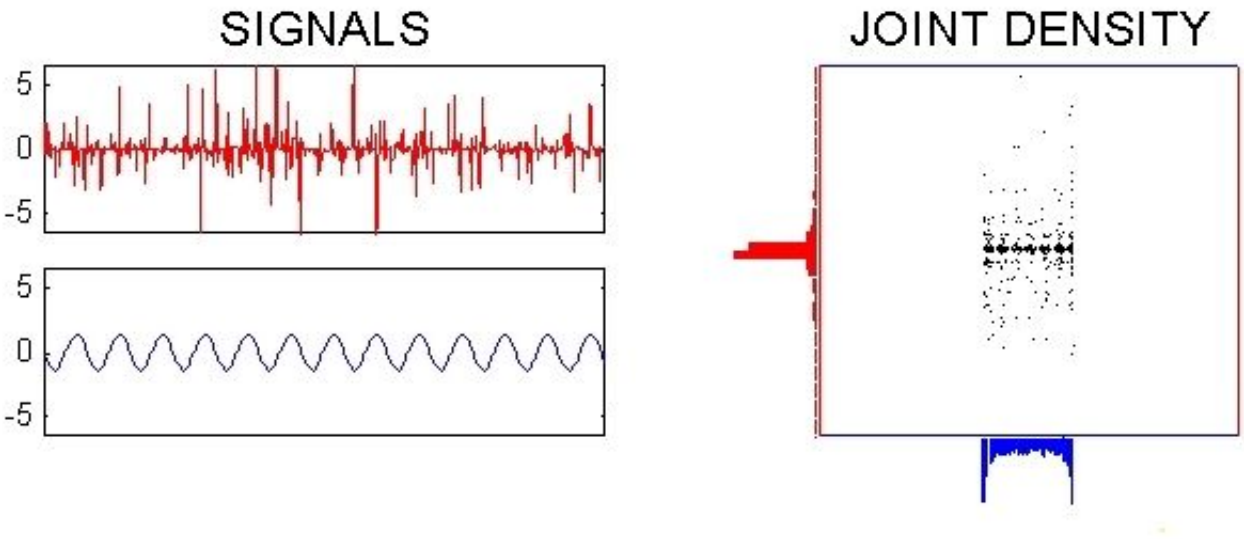
Separated signals after 3 steps of FastICA

ICA: Mixture Example



Separated signals after 4 steps of FastICA

ICA: Mixture Example



Separated signals after 5 steps of FastICA

ICA: Summary

- Learning can be done by PCA whitening followed kurtosis maximization.
- ICA is widely used for **blind-source separation**
- The ICA components can be used for features.
- Limitation: difficult to learn overcomplete bases due to the orthogonality constraint